Chemistry Department. Annual Report 1986

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Annual Report 1986 Chemistry Department

Edited by Jytte Funck, Elfinn Larsen and Ole John Nielsen

Risø National Laboratory, DK-4000 Roskilde, Denmark
March 1987

RISØ-M-2629

ANNUAL REPORT 1986
CHEMISTRY DEPARTMENT

Edited by Jytte Funck, Elfinn Larsen, and Ole John Nielsen

Abstract. This report contains a brief survey of the main activities in the Chemistry Department. All articles and reports published and lectures given in 1986 are presented. The facilities and equipment are mentioned briefly. The activities are divided into the following groups: radioisotope chemistry, analytical- and organic chemistry, environmental chemistry, polymer chemistry, radical chemistry, mineral processing, and general.

March 1987
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CONTENTS

This report contains a brief survey of the main activities in 1986 in the Chemistry Department including all articles and reports published and lectures given. The facilities and equipment are mentioned briefly.

The activities are divided into seven groups:

1. radioisotope chemistry
2. analytical- and organic chemistry
3. environmental chemistry
4. polymer chemistry
5. radical chemistry
6. mineral processing
7. general

MAIN ACTIVITIES

1. Radioisotope Chemistry

A part of the work is often performed in collaboration with researchers in the medical, geological, and archaeological fields from universities and hospitals. Certification work for the EEC Community's Bureau of Reference continues to be a major effort. Three papers were presented at The 7th International Conference on Modern Trends and Activation Analysis in Copenhagen.

A post-graduate study of the counting of rapidly decaying radioactive indicators has been completed in co-operation with the Technical University. A patent is pending, and the candidate was awarded the Angelo prize for 1986.

In collaboration with the Danish Isotope Centre instrumental neutron activation analyses and energy-dispersive X-ray fluorescence analyses have been made available to Danish industry. A staff vacancy has significantly delayed activity in this field.

In collaboration with the Niels Bohr Institute the production of ^{153}Gd has begun, and the development of a source of this isotope for the determination of bone mineral content by dual photon absorptiometry is in progress.

Industrial irradiation of silicon continues to be an activity of major concern, and a new irradiation facility for ingots up to 5" diameter was put into operation in April 1986.

The 7th international conference on Modern Trends in Activation Analysis was held on Hotel Scandinavia in Copenhagen on June 23rd-27th 1986. The conference was organized by The Radioisotope Laboratory. About 300 participants from 40 different countries attended the conference.

Fig. 1.1. Hilde Levi at the 7th Int. Conf. on MTAA, 1986.

Dr. Hilde Levi presented the first paper. In 1936 Hilde Levi together with the Nobel laureate Georg de Hevesy published the first article on activation analysis. A total of 175 papers were presented during the week, about half of the contributions as lectures and the remainder as posters. The subjects ranged from exploration of the solar system to localization of impurities in semiconductors. Advantageous discussions across geographical, cultural and political barriers took place

on different subjects such as improved methods for accurate estimation of trace elements, control of contamination and blanks, the correct use of reference materials etc. The posters showed examples from applications of activation analysis within the fields of archaeology, biology, geology, medicine, environmental and industial development. All the contributions are collected in two books compresing 1500 pages.

Fig. 1.2. The International Committee visiting the Radioisotope Laboratory during the conference MTAA in 1986.

An exhibition of instruments which are used in activation analysis measurements was well attended. The two firms Ortec and Nuclear Data held a reception the first day. The same evening an improvised meeting about experiments with measurements of radioactive fall out from the Chernobyl reactor accident was held in Hotel Scandinavia; 30 people participated.

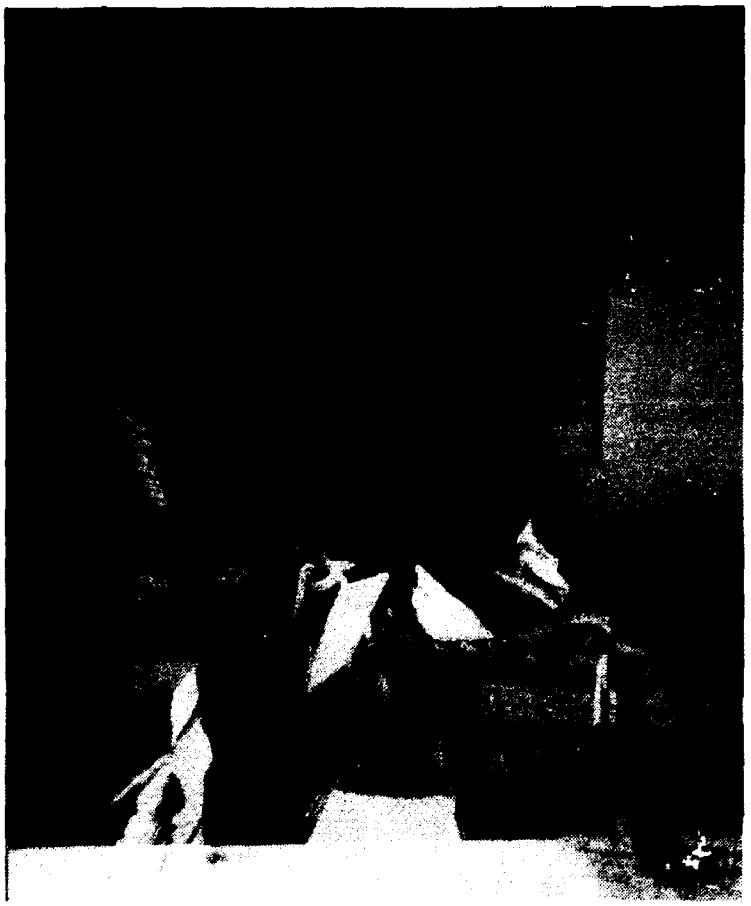

Fig. 1.3. The secretariat had some very busy days in connection with the MTAA conference.

The conference has received financial support from The National Science Research Council, The Thomas B. Thriges Fund, Tuborg Fund, Otto Mønsted Fund and Kraks Fund. Risø contributed with secretarial assistance.

Scientific Staff: K.Heydorn, Kirsten Andresen, Leif Højslet Christensen, Else Damsgaard, Ulf Jacobsen, Inge Overby Jensen, Jesper Jørgensen, Henrik Kalfod Nielsen.

Technical Staff: Lene Birch, Jytte Fritsche, Bo Gudmundsen, Jørgen Hanefeld-Møller, Ulrich Wagner Hansen, Jette Iversen, Henning Grandahl Jacobsen, Bente Jacobsson, Jytte Jakobsen, Bo Lars Jensen, Margit Elbek Jensen, Merete Larsen, Kirsten Madsen, Gitte Rasmussen, Mette Thomson, Børge Valentiner.

Guest Scientists: Vincent P. Guinn, Irvine, USA.
Marina Vasconcellos, Sao Paolo, Brazil.
Hilary Robotham, Jamaica
Namik K. Aras, Ankara, Turkey.

2. Analytical- and Organic Chemistry

In addition to the routine work within elemental analysis, chromatography, isotopic analysis and gas analysis several smaller commercial tasks are solved. Examples that may be mentioned are experiments to degas toxic compounds from laser-printed paper, and that the group worked two days at a drilling rig in the North Sea investigating air samples for an eventual content of particles and alkaline aerosols.

The demand for speciations of ions in aqueous solutions was fulfilled by installation of an ion chromatographic system. Cations and anions have been measured in water and in aqueous extraction from soil samples.

The work within the research area Physical Organic Chemistry has primarily been concentrated on the study of gas-phase pyrolytic

reactions and the continued development of the equipment for low-pressure pyrolysis reactions.

For gas kinetic studies, e.g. of surface-catalyzed reactions, a new and improved pyrolysis reactor, based on the principle of inductive heating, has been developed. In addition an extension of the pyrolysis facilities to include laser-induced reactions has been initiated. The basis for this facility is an old infra-red laser, which we have obtained from the Max Planck Institut für Quantenoptik in Munich. The development of the new pyrolysis facilities has been financed through a grant from the Danish National Science Council.

In connection with the development of the new pyrolysis facility, the fate of molecules in a low-pressure reactor was studied theoretically. The results was presented on the international pyrolysis conference in Reading, UK in September.

The possible influence of the surface in the pyrolysis process has received increased attention, as has the study of the pyrolysis-mass spectrometry interplay. The latter studies has resulted in a paper on rearrangement reactions of the nitromethan radical cation in the gas-phase.

The collaboration with Susanne Elbel (Hamburg) concerning pyrolysis studies on organometallic compounds continues. A collaboration with Henk Meuzelaar (Biomaterials Profiling Center, University of Utah) has been initiated. The project - Particulate Matter Pyrolysis - is financially supported by NATO.

The work with synthesis of compounds which are not commercially available continues. The interest in radiopharmica compounds is increasing. A laboratory for carrying out syntheses in larger scale has been established. The laboratory is placed in the buil-

ding of The Waste Treatment Plant, and the first synthesis has just been made successfully. The compound, 4,4',4''-triaminotriphenylcyanomethane, will be used for dosimetry measurements.

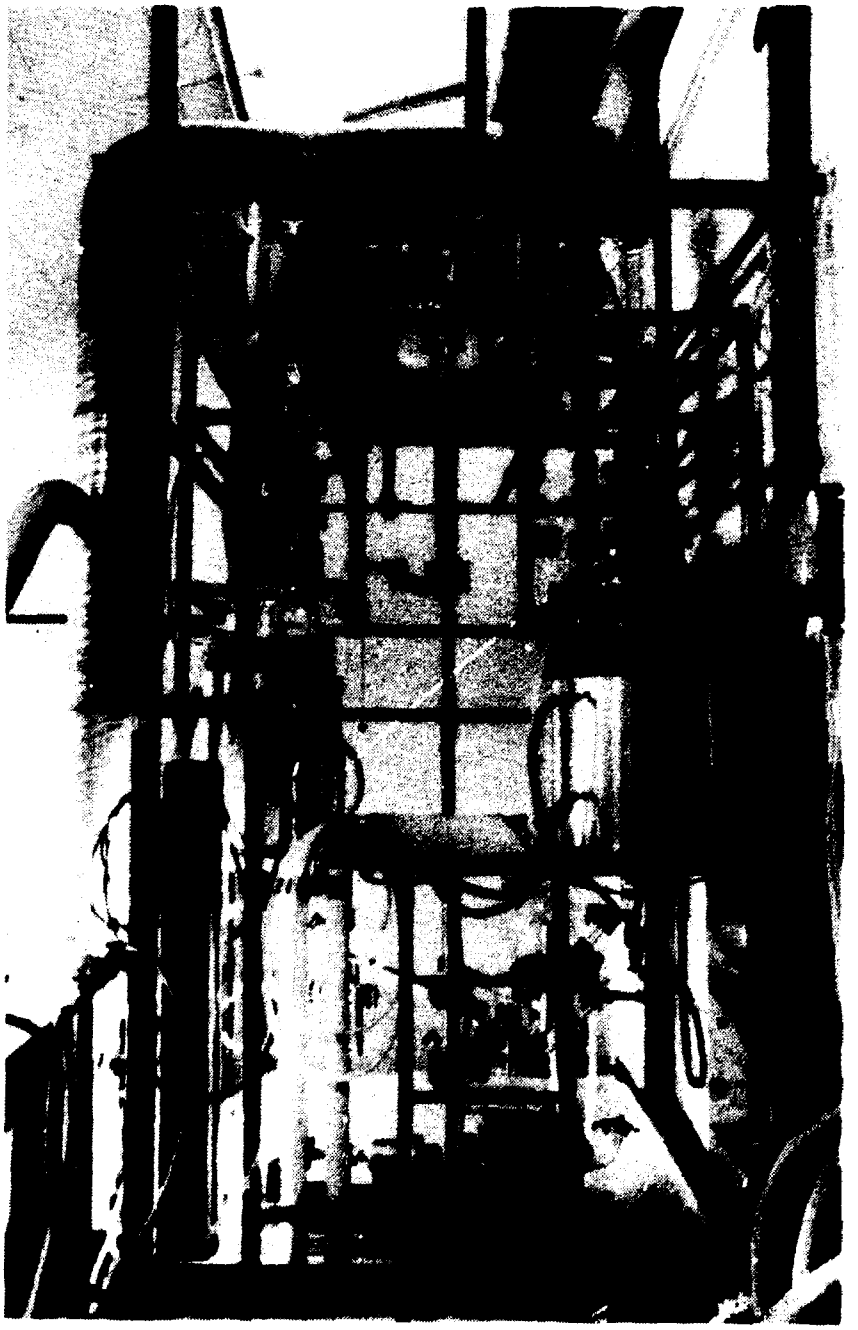

Fig. 2.1. Experiment set-up for large-scale syntheses.

The laboratory for hydrocarbon characterization is still expanding. A gas chromatographic system is now functioning and equipment for estimating density and molecular weight are being tested.

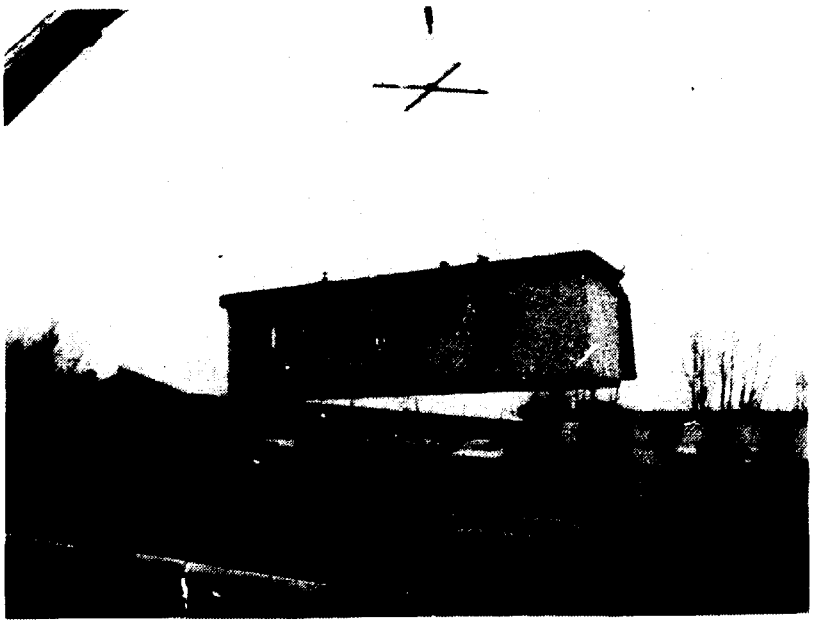

Fig. 2.2. The mineral analysis group moved to the Chemistry Department at the end of last year.

Scientific Staff: Lars Carlsen, Asger Baltzer Hansen, Helmar Kunzendorf, Elfinn Larsen, Per Solgaard.

Technical Staff: Karen Lis Christensen, Helge Egsgaard, Jytte Funck, Per Ingemann Jensen, Ole Jørgensen, Lis Vinther Kristensen, Susanne Petersen, Poul Sørensen, Niels Vinther.

Guest Scientist: Susanne Elbel, University of Hamburg.

3. Environmental Chemistry

Since the beginning of 1986 the activities of the Chemistry Department related to the environment has been carried out within the frame of a formalized Environmental Chemistry Group.

The Environmental Chemistry Group is involved in a variety of projects, primarily brought to the group by the members as a consequence of their previous affiliations. Hence, the Environmental Chemistry Group includes a) the geochemistry research, which includes experimental as well as theoretical work in areas as contaminant migration and geochemical modelling, b) the R&D carried out at the Waste Treatment Plant on nuclear waste, c) biological monitoring of metal deposition, d) environmental assessment of mining activities in Greenland, e) membrane chemistry, primarily ultra filtration, and f) atmospheric chemistry of polycyclic organic matter.

The major part of the activities of the Environmental Chemistry Group have been financed through external funding. In 1986 four major contracts within the nuclear research programme of the CEC have been signed.

Scientific Staff: Peter Bo, Knud Brodersen, Lars Carlsen, Bror Skytte Jensen, Ole John Nielsen, Torben Nielsen, Karen Nilsson, and Kim Pilegaard.

Technical Staff: Hanne Jensen, Gitte Larsen, Anne B. Nielsen, Jesper B. Rasmussen, Arne Vinther and Hanne Voss.

4. Polymer Chemistry

The viscoelastic properties of linear, amorphous polymers at short times were studied by Small Angle Neutron Scattering (SANS) experiments on a mixture of deuterated and hydrogenated polybutadiene with a molecular weight of 2×10^6. As neutrons are sensitive to the contrast between deuterium and hydrogen, changes in size due to a relaxation of deuterated polymer molecules can be followed in a SANS experiment. For the first time the chain contraction process was observed. This process is included in the Doi-Edwards model of viscoelastic properties of polymers, but previous experiments performed by other groups have been unable to show this surprising process.

A study of network defects in endlinked networks has been initiated. The dynamic mechanical properties of endlinked networks prepared from monodisperse dimethylsiloxane and butadiene prepolymers will be used to determine the number of free chain ends in the polymer networks. Hopefully, these experiments will settle the current dispute about the contribution of chain entanglement to the modulus of rubber networks.

The construction of a vacuum line has been completed. This enables us to make different monodisperse polymers with special functional groups.

The presence of high molecular weight components in insulin solutions approved for clinical use were studied by size exclusion chromatography (SEC) using a laser light scattering detector. A polymer of insulin with a molecular weight of more than 10^6 (> 160 insulin molecules) has been isolated and the characterisation of the aggregate initiated. The amount of insulin polymer was influenced by the pH of the insulin solution as well as the storage conditions (time and temperature).

The studies of chain mobility in linear and crosslinked polymer networks and the structures of macromolecules in aqueous soltion will be intensified due to a grants from the Danish Technical Research Council and the National Agency of Technology.

The installation of an advanced mechanical spectrometer Rheometrics RMS 800 (see Fig. 4.1.) was financed by the National Agency of Technology. The RMS 800 measures mechanical properties in dynamic and steady of a large variety of materials, including thermoplastics, thermosets, rubbers, suspersions, polymer solutions etc. The instrument will be used in different research projects:

a) Network defects in three-dimensional networks
b) Soft composite materials with tunable energy-absorbing properties
c) Characterisation of flow properties of polyethylene with the aim of designing better tools for the extrusion of high-voltage cables
d) Characterisation of drilling mud.

The instrument will also be available to Danish industry.

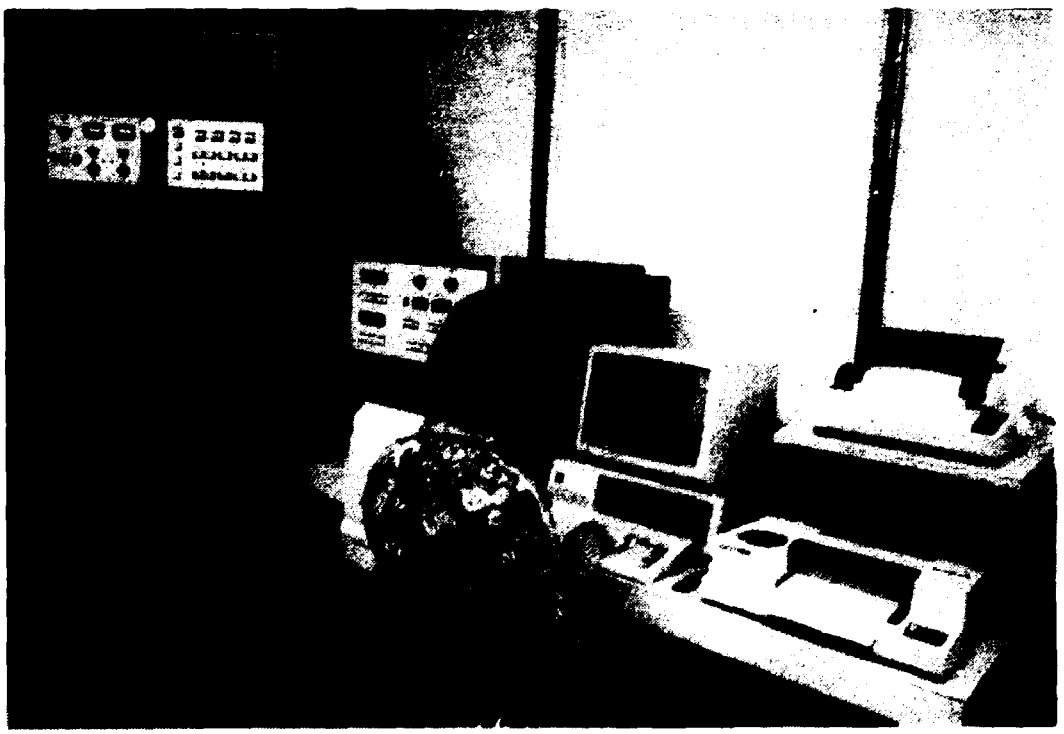

Fig. 4.1 The newly installed Rheometer.

During the period, HPLC and SEC techniques were used in a number of projects, some of them as contract work for private firms:

- Characterisation of polymethylmethacrylate with extremely high molecular weight.
- Development of a thermoplastic rubber for medical use.
- Long-term stability of polyethylene.
- Characterisation of different heparin preparations.

Furthermore, the work with sterilization technology was continued, mainly on an advisory basis for private firms and public authorities.

Fig. 4.2 Vagn N. Handlos obtained his doctorate and received the "doctor ring" of the Chemistry Department.

Scientific Staff: Kristoffer Almdal, Vagn Neerup Handlos, Søren Hvidt, Søren Hvilsted, Ole Kramer, Walther Batsberg Pedersen.

Technical Staff: Lotte Hansen, Lene Hubert.

5. Free Radical Chemistry

The two main research activities undertaken by the free radical chemistry group are Gas Phase Kinetics and Transient Resonance Raman Spectroscopy.

The aim of the experimental work within gas phase kinetics is to investigate chemical reaction mechanisms and measure rate parameters for elementary reactions which are of importance in atmospheric chemistry and combustion processes. In the field of atmospheric chemistry substantial experimental work has been carried out under the CEC Environmental Research Programme, Contract No. ENV-872-DK. The final Report describing our studies of SO_2 oxidation initiated by OH, HO_2, and CH_3O_2 is available from the Risø Library. In the field of combustion chemistry we have studied UV-spectra and kinetics of ethyl and ethylperoxy radicals which are the main intermediates in the low-temperature oxidation of ethane. Professor Emil Ratajczak from the University of Wroclaw has joined us in a combustion research program EFP-85 supported by the Danish Ministry of Energy. Our contribution has been studies of free radical reactions in the oxidation of propane.

We are also engaged in the CEC-sponsored European Programme on Combustion Kinetics, Contract No. EN3E-0095-DK (B). Our work has been concentrated on studies of unsaturated hydrocarbon radicals which play an important role in the formation of soot and aromatic hydrocarbon products. In the first periodic report we have decribed our spectrokinetic studies of vinyl radicals. In collaboration with Christopher Anastasi from University of York we have investigated different source reactions for the hydroxymethyl radical and we have recorded a complex vibronic spectrum in the range of 200-300 nm which has not been observed

previously. We have studied the self-reaction of CH_2OH as well as the reaction with oxygen. Spectroscopic work on the isotopic radical species CD_2OD and CH_2OD is in progress and the results may allow us to carry out a complete analysis of the spectral features. Quantum-mechanical ab initio calculations on the electronic ground state and several excited states of CH_2OH have been carried out by Sten Rettrup at the H.C. Ørsted Institute in Copenhagen.

There is a considerable interest in studies of the chemical reaction mechanisms involved in the interconversion of nitrogen oxides in the troposphere. In addition to the well-known members of the NO_x-family, i.e. NO and NO_2, there exists a more labile species NO_3, the nitrate radical that may play an important role as "night-time oxidant" for various organic trace species in the trcposphere. We have studied the simultaneous formation of O_3 and NO_3 which are produced by pulse radiolysis of O_2/NO_2 mixtures. The time profiles of O_3 and NO_3 were studied by monitoring the transient absorption signals at 255 and 662 nm, respectively. Work is in progress to analyse the experimental results by a computer modelling of the kinetic features taking into account simultaneous reactions between all of the species which are present in the irradiated gas sample, i.e. O, O_2, O_3, NO, NO_2, NO_3 and N_2O_5. The reaction $F + HNO_3 \rightarrow HF + NO_3$ appears to be an ideal source reaction providing high yields of NO_3 radicals which are very long-lived in the absence of reactive impurities. We are now in a good position to study the reactions of NO_3 with other radicals, e.g. OH and HO_2 as well as reactions with various organic compounds which occur in the natural and polluted troposphere.

The use of F-atoms as a precursor of secondary radicals via abstraction reactions $F + RH \rightarrow HF + R$ has been very successful. Because of our interest in studies of the consecutive

reactions R + O_2 -> RO_2 we found it necessary to study also the reaction F + O_2 = FO_2 which may compete with the formation of the organic peroxy radicals, RO_2. Our preliminary results show that the back reaction is relatively fast even at room temperature which indicates a low bond energy D(F-O_2). Work is in progress to determine the heat of formation of FO_2. Reactions of OH with organic sulfides and di-sulfides has been the main subject of our collaboration with Howard Sidebottom at University College in Dublin. The collaboration continues with studies of chemical transformations of organosulphur compounds of interest to atmospheric chemistry. A preliminary investigation of SO_2/H_2O interactions in the gas phase has been carried out by FTIR spectroscopy in collaboration with Flemming Nicolaisen at the H.C. Ørsted Institute in Copenhagen. Attempts are being made to analyse the intermolecular force fields which are responsible for the observed line broadening.

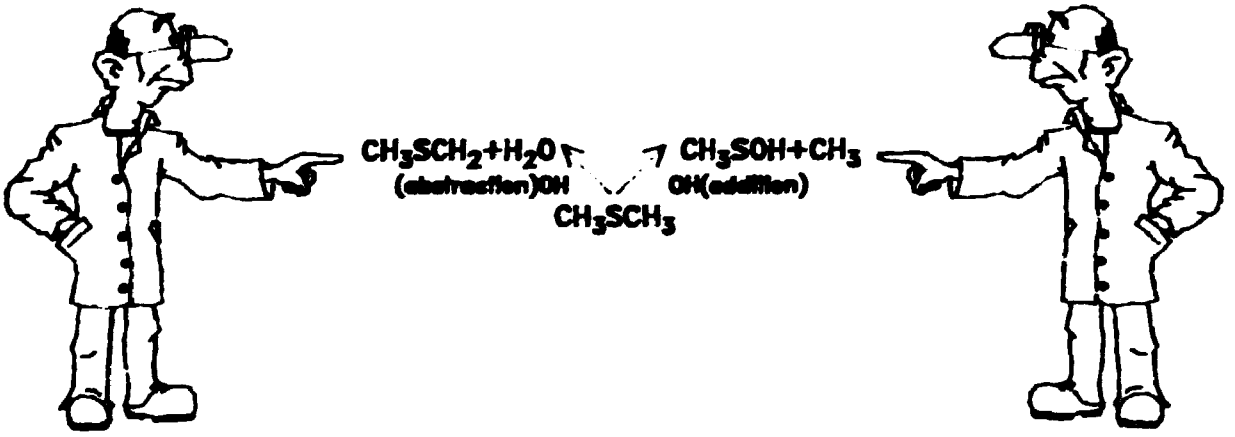

Fig. 5.1 The reaction of OH with CH_3SCH_3 has two pathways.

For the Raman group 1986 has been characterized by the twelve-month construction period of our laboratory for time-resolved resonance Raman measurements. This construction has now been completed, and our experimental set-up is again active in

January 1987. An important consequence of the new laboratory configuration is that the experimental set-ups for Raman spectroscopy and gas radiolysis now are independent of each other. This has increased the capacity of the entire Radical Chemistry group and has facilitated the work procedures greatly.

Besides time-resolved resonance Raman measurements of excited states of polyenes, during 1986 we have worked with the vibrational spectroscopy of polyene ground states, in collaboration with the FTIR and Raman groups at the H.C. Ørsted Institute (HCØ), Copenhagen University, using the instrumentation at HCØ.

Along with the construction of new experimental facilities at Risø and the experiments at HCØ, a large number of manuscripts were written and submitted for publication. Finally, Frans W. Langkilde has written and submitted his Ph.D. Dissertation.

Scientific Staff: K.B.Hansen, Niels Henrik Jensen, Frans W. Langkilde, Ole John Nielsen, Palle Pagsberg, Alfred Sillesen, and Robert Wilbrandt.

Technical Staff: Jette Munk and Preben Genske.

Guest Scientists: Professor Emil Ratajczak, University of Wroclaw, Poland.
Howard Sidebottom, University College, Dublin, Ireland.
Christopher Anastasi, University of York, England.
Christian Lohse, University of Odense, Denmark.

6. Mineral Processing

The section works in areas of extraction of elements from ores, conditioning of tailings and other waste materials, synthesis of silicates, and in general processing involving the use of high-temperature autoclaves. Chemistry, engineering and environmental science are integrated in this section. Current projects include gold extraction and hazardous waste treatment.

Scientific Staff: Jørgen Jensen, Emil Sørensen, Torkild Lundgaard, Jette Paulsen, Belinda Bjerre.

Technical Staff: Helle Krogh, Jette Posskov, Sv.Kr. Olsen, Tomas Fernqvist.

7. General

The Department accomplishes chemical analysis and services for other departments at Risø and on a commercial basis for customers outside Risø.

The Isotope Laboratory has continued to fulfil its commitment as the sole producer of neutron-irradiated materials for technical and scientific purposes in Denmark. The collaboration with the Isotope Pharmacy has proceeded in the production of radiopharmaceuticals for medical diagnostics, and lately in preparing the documentation for a ^{131}I-labelled cellulose compound. Radioisotope production mainly for scientific research has continued. As a supplement to the α, β, and γ demonstration sources for educational purposes, supplied to the Nordic countries, a ^{226}Ra source for continuous cloud chambers is available.

The handling and disposal of radioactive wastes from Risø and other users of radioactive isotopes are taken care of at The Waste Treatment Plant.

During the year several laboratories have been renovated and a new meeting room has been built.

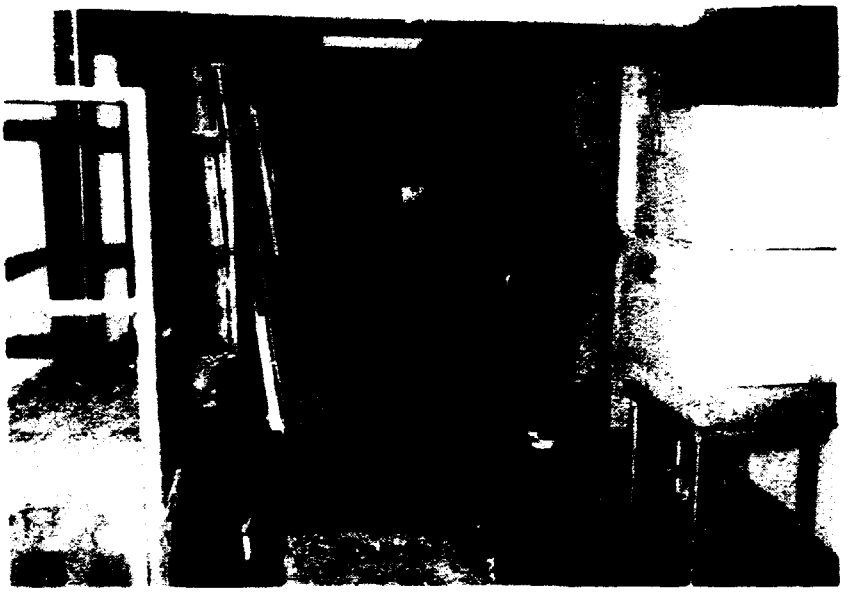

Fig. 7.1. Renovating of the laboratories.

Fig. 7.2. The new meeting room in The Chemical Laboratory.

A technical staff takes care of typing, workshop, laundry, radioactive cleaning, etc.: Aase Neve Larsen, Kirsten Bay, Ingrid M. Pedersen, Annie C.S. Andersen, Jytte Green, Ellen M. Jensen, Esther Andersen, Inger Jacobsen, Fini Lindskou, Svend Nielsen, Knud Larsen, Erling Christensen, Bent Villumsen, Elsebeth G. Jensen, O. Sølling-Hansen, Bent Nielsen, Jørgen Larsen, Sven Jensen, Børge Rasmussen, Signe Hansen, Birthe I. Hansen, Birthe N. Andersen, Pedro Breschiani, Nina Thomsen, Ruth Ågesen, Svend Erik Kerchhoff.

Risø's Chemistry Department includes four geographically separated sections: The Chemical Laboratory, The Radioisotope Laboratory, The Waste Treatment Plant, and The Mineral Processing Plant.

The staff of The Department consists of 35 members with academic degrees, 4 Ph.D. students and 62 technicians.

PUBLICATIONS

MODERN TRENDS IN ACTIVATION ANALYSIS, COLLECTED PAPERS.

Vol.1 Methodology pp. 1-708
Vol.2 Applications pp. 709-1437

K.Heydorn.

Isotope Division, Risø, 1986. ISBN 87-550-1207-8

Fifty years ago the use of a nuclear reaction in analytical chemistry was unheard of, and only George de Hevesy and other eccentrics at the Niels Bohr Institute of Theoretical Physics could come up with such an idea. For a number of years the method remained an oddity, and only ten papers were published during the first decade; but the availability of nuclear reactors and charged particle accelerators to non-physicists after the second world war stimulated interest in the development of activation analysis as a new discipline.

This formed the basis for organizing an international conference in 1961 at Texas A&M University, which was named Modern Trends in Activation Analysis, and which became the first of a series of conferences devoted to activation analysis. An International Committee was created, and subsequent conferences were held at College Station (1965), Washington (1968), Paris (1972), München (1976), and Toronto (1981).

The incredible development from the home-made string and sealing wax equipment used in the original work of 1936 to the sophisticated wizardry commercially available today, has paved the way for the application of activation analysis in virtually all branches of science. More than half of the papers presented to the MTAA-7 Conference bear witness to this close association with scientific endeavour to solve problems in archaeology, biology, geochemistry etc.

Perhaps even more surprising is that the methodology of activation analysis continues to develop, and almost half of the papers presented to the MTAA-7 demonstrate how the basic principle can be combined with new techniques or methods developed in other fields like physics and chemistry, mathematics, statistics, chemometrics etc. This illustrates that the discipline of activation analysis is still a scientific area which maintains a momentum of its own and is capable of renewing itself in every new generation of scientists.

We are proud that Denmark was chosen to host this conference and thereby contribute to the interdisciplinary exchange of ideas and friendship among scientists from all over the world. Colleagues from 53 countries have registered their interest in attending, and abstracts of 280 papers were submitted for presentation at the MTAA-7 Conference. Unfortunately, not everyone who wishes to attend the MTAA-7 will be able to do so, and not every abstract will result in a formal publication. But the enthusiasm and the inspiration are here, and the field of activation analysis remains as active as ever - even though it has reached maturity.

Kaj Heydorn Hilde Levi

PRENATAL DIAGNOSIS OF MENKES' SYNDROME BY DIRECT COPPER ANALYSIS OF TROPHOBLASTIC TISSUE.

N.Horn, F.Søndergaard, E.Damsgaard and K.Heydorn.

in First Trimester Fetal Diagnosis.
Springer, Heidelberg, 1985. 251-255.

Menkes' syndrome is a congenital disruption of copper metabolism transmitted as an X-linked recessive trait and characterized by increased copper accumulation in multiple cell types in the body and in culture (Horn 1976; Goka et al. 1976; Beratis et al. 1978; Camakaris et al. 1980). The excess of copper serves as a useful diagnostic marker. Incorporation of labelled copper into cultured amniotic fluid cells is now routinely used for selective prenatal diagnosis (Horn 1981). Copper incorporation into cultures obtained from affected male fetuses is, however, negatively correlated with the gestational age at amniocentesis, and after the 18th week of gestation, the risk of misclassification is significant (Horn 1983).

The accumulation of excessive amounts of copper in the placental tissue of affected male fetuses is useful as a verification of the prenatal diagnosis (Horn 1981; Damsgaard et al. 1983). Analysis of a spontaneous abortion in the 8th week of gestation has shown that affected fetuses also accumulate excessive amounts of copper in the placenta early in the pregnancy (unpublished data). The principal site of copper accumulation appears to be the trophoblast, which has a transcellular transport function (Horn 1981, 1984). Since chorionic villi contain a high proportion of trophoblastic cells they should be useful in the prenatal diagnosis of Menkes' syndrome. This paper reports the successful implementation of this marker in the first trimester prenatal diagnosis of Menkes' syndrome in four at-risk pregnancies.

SYNTHESIS OF PRECISION FOR THE CERTIFICATION OF PHOSPHORUS IN BIOLOGICAL MATERIALS BY INAA.

E.Damsgaard and K.Heydorn.

in Modern Trends in Activation Analysis.
Isotope Division, Risø, 1986. 671-676. ISBN 87-550-1207-8

The β-emitter ^{32}P was used to determine total phosphorus by INAA in Skim Milk Powder RM 63, a material now certified by tne EEC Bureau of Reference (BCR). Samples and comparator were irradiated in the Danish reactor DR 3. One month later the samples were dissolved in water and aliquots counted with a GM end-window counter using absorber thicknesses of zero to 400 mg/cm^2. The Synthesis of Precision was introduced to find the absorber best suited for discriminating against other β-emitting isotopes and at the same time giving maximum precision.

COPPER-MEASUREMENT IN A MUSCLE-BIOPSY. A POSSIBLE METHOD FOR POSTMORTEM DIAGNOSIS OF MENKES DISEASE.

T.Tønnesen, G.Müller-Schauenburg, E.Damsgaard and N.Horn.

Clinical Genetics. 29 (1986) 258-261.

A 5-month-old boy showed severe delay in mental and motor development. His hair was normal. He died at 18 months from bronchopneumonia. Autopsy of the brain revealed meningo-cerebral angiodysplasia with tortuous vessels at the surface of the brain. This raised a suspicion of Menkes disease.

A muscle-biopsy, the only remaining tissue from the patient, showed an increased copper-content, thus corroborating the suspicion of Menkes disease. Copper uptake studies on 2 independent repeatedly tested fibroblast-cultures from the mother gave normal values in 4 and elevated levels in three tests. Such a pattern is often seen in carriers of Menkes disease. Furthermore one of the test values was above the critical limit. Just one value above this limit for females from families with Menkes disease will unequivocally classify a woman as a carrier irregardless of her genetic risk.

This is to our knowledge the first time copper-measurements in tissues have been used to establish a post-mortem diagnosis of Menkes disease.

QUALITY ASSURANCE IN THE DETERMINATION OF OVERLAPPING PEAK AREAS.

Leif Højslet Christensen and Kaj Heydorn.

in Modern Trends in Activation Analysis.
Isotope Division, Risø, 1986. 551-559. ISBN 87-550-1207-8

The ability of different computer programs to yield accurate peak areas in statistical control in the case of partially overlapping photopeaks has been tested by the Analysis of Precision. A modified Covell method, two commercially available peak fitting programs from Nuclear Data and Ortec, and the SAMPO80 program were used to evaluate the 843.8 keV peak area in the 843.8/846.6 keV doublet of ^{27}Mg and ^{56}Mn produced by thermal neutron activation of a candidate biological reference material to be certified for magnesium. The best performance was given by the Ortec program, but a modified SAMPO80 performed almost as well. The modified Covell program gave reliable results, but with poorer precision.

INSTRUMENTAL NEUTRON ACTIVATION ANALYSIS TECHNIQUE USING SUBSECOND RADIONUCLIDES.

H.K.Nielsen and J.O.Schmidt.

in Modern Trends in Activation Analysis.
Isotope Division, Risø, 1986. 749-753. ISBN 87-550-1207-8

The fast irradiation facility Mach-1 installed at the Danish DR 3 reactor has been used in boron determinations by means of Instrumental Neutron Activation Analysis using ^{12}B with 20-ms half-life.

The performance characteristics of the system are presented and boron determinations of NBS standard reference materials as well as fertilizer materials are compared by literature value and spectrophotometric measurements, respectively. In both cases good agreement is obtained.

RATE OF REACTION OF DIMETHYLMERCURY WITH OXYGEN ATOMS IN THE GAS PHASE.

E.Lund Thomsen and Helge Egsgaard.

Chemical Physics Letters 125 (1986) 378-382.

Dimethylmercury is a pernicious poison. It is lethal in comparatively small doses and can cause strongly disabling chronic poisoning [1,2].

The presence of dimethylmercury in the atmosphere has been shown by several workers [3], and a considerable interest in its atmospheric fate can be noted regarding its role as a potential hazard as well as in connection with the evaluation of man-made perturbations of the natural mercury cycle.

The work reported in the present study deals with measurements of the reaction rate of dimethylmercury with O atoms at room temperature as well as the determination of some reaction products. The experimental method used is the fast flow reactor technique with EPR and mass spectrometric (MS) detection.

TECHNIQUES IN GAS-PHASE THERMOLYSES

PART 7. DIRECT SURFACE PARTICIPATION IN GAS-PHASE CURIE-POINT PYROLYSIS: THE PYROLYSIS OF PHENYL AZIDE.

Helge Egsgaard and Lars Carlsen.

Journal of Analytical and Applied Pyrolysis, 10 (1986) 83-87.

The possible direct participation of the hot reactor surface in the formation of pyrolysis products was elucidated through the pyrolytic decomposition of phenyl azide. It is demonstrated that the intermediate phenyl nitrene generated reacts with elemental carbon at the filament surface, leading eventually to benzonitrile. The importance of well defined surfaces is discussed.

LOW PRESSURE PYROLYSIS/MASS SPECTROMETRY. STRATEGIES FOR DISCLOSING REACTION PATHWAYS.

Helge Egsgaard and Lars Carlsen.

in Advances in Mass Spectrometry
Ed. J.F.J.Todd Wiley, New York (1986) 1311-1312.

Application of mass spectrometry as an analytical technique for gas phase pyrolytic reactions offers an excellent opportunity for elucidating reaction mechanisms. In this connection the application of stable isotopes appears as unique. Even though the potential of isotopic labelling for mechanistic studies is well recognized, the method becomes increasingly attractive in connection with real-time-analysis of e.g. isomerizations, the thermally induced 1,3 alkyl shift in carboxylic acid esters being a typical representative.

Analogous to the known rearrangement of thiono esters into the thermodynamically more favourable thiolo isomers [1], pyrolysis of ^{18}O-labelled methylacetate unequivocally was demonstrated to result in a 1,3 methyl group migration [2]. Surprisingly, however, similar studies of the ^{34}S-labelled methyl dithioacetate revealed the absence of a 1,3 sulfur to sulfur methyl group migration [3].

In the latter case hydrogen/deuterium exchange of labile hydrogen atoms (-OH, -SH, -NH) by molecule - wall interactions has proved to be of diagnostic importance [3]. Hence, the intermediacy of the enethiolized tautomer in the pyrolysis of methyl dithioacetate has recently been demonstrated by co-pyrolysis with D_2O [3], i.e. H-D exchange was observed as a result of interaction between the SH moiety and surface bound D_2O.

In Figure 1 the molecular ion regions before and after pyrolysis (1043 K) of methyl dithioacetate are shown together with partial collision activation mass spectra of the m/z 107. The increased intensity of the m/z 60 unambiguously demonstrates the incorporation of deuterium in the thioacetyl group [3].

GASFASE PYROLYSE.

Lars Carlsen and Helge Egsgaard.

Risø Nyt, Marts 1986, 8.

Pyrolyse, d.v.s. reaktioner initieret af høje temperaturer (typisk 500-1500°C), er en vidt udbredt teknik inden for meget forskellige områder af kemien, spændende fra ren fysisk kemi over fysisk organisk/uorganisk kemi og fremstilling af organiske/uorganiske forbindelser i mindre målestok, til karakterisering af for eksempel jordprøver, levnedsmidler, plastmaterialer samt ved biologiske, medicinske og retskemiske undersøgelser.

TRIPHENYL PHOSPHATE ALLERGY FROM SPECTACLE FRAMES.

Lars Carlsen, Klaus E.Andersen and Helge Egsgaard.

Contact Dermatitis 15 (1986) 274-277.

A case of triphenyl phosphate allergy from spectacle frames is reported. Patch tests with analytical grade triphenyl phosphate, tri-*m*-cresyl phosphate, and tri-*p*-cresyl phosphate in the concentrations 5%, 0.5% and 0.05% pet. showed positive reactions to 0.05% triphenyl phosphate and 0.5% tri-*m*-cresyl phosphate, but no reaction to tri-*p*-cresyl phosphate. Gas chromatography of the tricresyl phosphate 5% pet. patch test material supplied from Trolab showed that it contained a mixture of a wide range of triaryl phosphates, including 0.08% triphenyl phosphate which is above the threshold for detecting triphenyl phosphate allergy in our patient.

ISOMERIZATIONS OF THE NITROMETHANE RADICAL CATION IN THE GAS PHASE.

Helge Egsgaard, Lars Carlsen and Susanne Elbel.

Ber. Bunsenges. Phys. Chem. 90 (1986) 369-374.

Elementary Reactions / Ionization / Isotope Effects / Mass Spectrometry / Thermodynamics

The concurrent isomerizations of the nitromethane radical cation to its *aci*-nitromethane and methylnitrite isomers, respectively, has been established based on metastable ion studies and collision activation mass spectrometry. The energy diagram for the ionized nitromethane/*aci*-nitromethane tautomeric system has been determined; the *aci*-nitromethane tautomer was found to be the more stable species by ca. 0.95 eV. Attempts to generate the neutral gaseous *aci*-nitromethane tautomer by low pressure pyrolysis are summarized.

EVIDENCE OF GASEOUS $AsCl_4F$ FROM $AsCl_4^+AsF_6^-$ BY U.P.S. AND F.I.M.S. INVESTIGATIONS.

Susanne Elbel, Gerda Rünger, Helge Egsgaard and Lars Carlsen.

J. Chem. Research (S) (1986) 294-295.

We report the production of gaseous $AsCl_4F$ by heating $AsCl_4^+ AsF_6^-$, and its characterization by u.v. photoelectron spectroscopy and field-ionization mass spectrometry.

THE INTERACTION OF RADIONUCLIDES WITH NATURALLY OCCURRING ORGANICS.

L.Carlsen.

in The Effects of Natural Organic Compounds and Microorganisms on Radionuclide Transport.
Ed. A.B.Muller. OECD-NEA, RWN-6 (1986) 77-88.

Interactions between naturally occurring organics as humic and fulvic acids and radionuclides have been reviewed. The radionuclides considered in the present study comprise cesium, strontium, cobalt, nickel, europium, as well as the actinide elements. The different possible reactions are discussed. The study lead to the conclusion that a basic knowledge of the single possible reactions, e.g. complex formation, exchange reactions, sorption phenomena, is of extreme importance, in order possibly to predict the role of organics on the migration of radionuclides in the geosphere.

SPECIFIC INVESTIGATIONS RELATED TO SALT ROCK BEHAVIOUR.

L.H.Vons, A.Zelikson, L.Charo, H.Gies, C.J.Spiers, J.P.A.Roest, J.Gramberg and L.Carlsen.

in Radioactive Waste Management and Disposal.
Ed. R.Simon. Cambridge University Press, (1986) 434-449.

In this paper results are given of work in various countries in rather unrelated areas of research. Nevertheless, since the studies have been undertaken to better understand salt behaviour, both from mechanical and chemical points of view, some connection between the studies can be found. In the French contribution (A) the geological conditions have been investigated that might promote or prevent the formation of salt domes from layers in view of possible use of the latter type of formation.

This was done theoretically by the finite element method, and a start was made with centrifuge tests. The density of a number of samples from salt and overburden from the Bresse basin was measured and it was shown that a favourable condition exists in this region for waste disposal.

In the German contribution (B) various subjects are touched upon, one being the effect of water on the mobility in the early stages of salt dome formation. Evidence was found for an anisotropy in salt.

One Dutch contribution (C) describes results of studies on the effect of small amounts of water on the rheology of salt. The results imply that flow laws obtained for salt at rapid strain rates and/or low confining pressure cannot be reliably extrapolated to predict the long term behaviour of wet or even very dry material under natural conditions.

Preliminary results on the effect of water upon ion-mobility indicate a certain pseudo-absorptive capacity of salt e.g. for Sr.

Another Dutch contribution (D) presents results of laboratory and in-situ measurements at ambient temperatures in the Asse-mine, with an acoustic method to detect the extension of cracks in stress-relieved locations, such as gallery walls etc.

A somewhat related type of work is presented in the Danish contribution (E) where the absorptive capacity of powdered salt for a range of radio-nuclides of different valency was measured both for pure salt and salt with addition of hematite and anhydrite impurities.

CU (I) SUPPORTED ISOTOPIC EXCHANGE OF ARYLBOUND IODIDE, NEW FUTURE FOR FAST HIGH YIELD LABELLING.

J.J.R.Mertens, W.Vanryckeghem and L.Carlsen.

in Progress in Radiopharmacy.
Eds .P.H.Cox, S.J.Mather, C.B.Sampson and C.R.Lazarus.
Martinus Nijhoff Publishers, Dordrecht (1986) 101-109.

The labelling methods for the radioiodination of aryl-compounds, based on nucleophilic isotopic exchange, which have been described until now, can be summarized as follows: Cu(II) catalysed reactions (1-6) $(NH_4)_2SO_4$ solid state transfer methods (6-8) and reactions occurring in liquid phase (pseudo melt) in absence of any catalyst (6,9,10). These methods were shown to give low and/or poorly reproducible labelling yields with the generation of labelled by-products and/or radioiodine. This implies that time consuming and costly purifications are required when the patient friendly but expensive short-lived I^{123} is involved.

This paper describes a new chemical approach to the nucleophilic isotopic exchange of arylbound iodine, based on the use of Cu(I) in an acidic medium in the presence of an excess of reducing agent, such as Sn(II) and ascorbic acid ⊕. This method has been applied with success to the radioiodination of iodo-arylcompounds of great interest in nuclear medicine such as: N-isopropyl-p-iodoamphetamine (IAMP), m-iodobenzyl-guanidine (MIBG) and o-iodohippuric acid (hippuran). Labelling yields of ∿99% have been obtained and this chemistry has permitted the development of genuine kit-form labelling methods.

THE INFLUENCE OF CHEMICAL REACTIONS ON THE MOBILITY OF RADIONUCLIDES IN THE TERRESTRIAL ENVIRONMENT.

Lars Carlsen, Ole John Nielsen, Peter Bo and Conny Ditlevsen.

Risø-M-2533 (1986) ISBN 87-550-1158-6

The influence of the kinetics of chemical and physico-chemical reactions on the mobility of radionuclides in the terrestrial environment has been studied theoretically by application of the COLUMN2 computer code. A variety of reaction systems has been analyzed comprising:

$A \rightarrow B$

$A \rightarrow B \rightarrow C$

$A \rightleftarrows B$

$A \rightleftarrows B \rightarrow C$

$A \rightleftarrows B \rightleftarrows C$

$A + X \rightarrow B$

$A + B \rightleftarrows C$

$A + B \rightleftarrows C + D.$

The study unequivocally discloses the importance of the chemistry in controlling the migration behaviour of contaminants, e.g. radionuclides in the terrestrial environment. The analyses suggest the necessity of studying possible geochemical reaction in detail, including both retention characteristics as well as reaction kinetics.

RETENTION OF RADIONUCLIDES IN HALITE AND ANHYDRITE.

Lars Carlsen and Dorte Platz.

European Appl. Res. Rept.- Nucl. Sci. Technol. 7 (1986) 539-575.

The interaction between a series of radionuclides, comprising $^{134}Cs^{+}$, $^{85}Sr^{2+}$, $^{60}Co^{2+}$, $^{154}Eu^{3+}$, $^{241}Am^{3+}$, and ^{99}Tc (as TcO_4^-) and halite (NaCl) and anhydrite ($CaSO_4$), respectively, has been investigated.

It appears that europium and americium as chloro-complexes MCl_2^+ (M = Eu, Am) interact with the halite surface apparently forming solid europium/americium chloride (MCl_3) moieties, which are desorbed only with difficulty.

Batch-type experiments revealed distribution coefficients in the order of 20 and 75 for europium and americium, respectively.

Impurities in the halite, such as hematite or anhydrite strongly increase the sorption efficiency. In these cases also cobalt, and to a minor extent cesium and strontium, was found to be sorbed.

Anhydrite was found to sorb all metal cations studied. The sorption efficiency was found to be dependent of the sodium chloride solution. Typically, the highest sorption efficiency for anhydrite was found at intermediary sodium chloride concentration levels (3 - 5 M), whereas high or low levels resulted in a decreased efficiency. At NaCl concentrations below ca. 2 M anhydrite was converted into gypsum.

DETERMINATION OF 2-NITROFLUORANTHENE AND 2-NITROPYRENE IN AMBIENT PARTICULATE MATTER: EVIDENCE FOR ATMOSPHERIC REACTIONS.

T.Nielsen and T.Ramdahl.

Atmospheric Environment. 20 (1986) 1507-1509.

Pitts *et al.* (1985) have presented a very interesting paper containing important news on atmospheric reactions of polycyclic aromatic hydrocarbons (PAH) and the presence of their mononitro derivatives in urban air at summer-time conditions. We have earlier (Nielsen *et al.*, 1984) identified 2-nitropyrene (NP), 3- and 8-nitrofluoranthene (NF) (the latter tentatively), and five other mononitro-PAH in rural air at winter-time conditions with low concentrations of photochemical air pollutants and NO_2.

Pitts *et al.* (1985) only found traces of 3-NF in one of their samples, in all samples the main isomer identified was 2-NF, which eluted immediately ahead of 3-NF on the GC-column used (see also Ramdahl *et al.*, 1985). We have therefore reinvestigated our earlier results. This revealed that the compound identified as 3-NF in our sample collected at Risø in Denmark was actually 2-NF.

DETERMINATION OF BASIC AZAARENES AND POLYNUCLEAR AROMATIC HYDROCARBONS IN AIRBORNE PARTICULATE MATTER BY GAS CHROMATOGRAPHY.

Torben Nielsen, Per Axel Clausen and Finn Palmgren Jensen.

Analytica Chimica Acta. 187 (1986) 223-231.

Polynuclear aromatic hydrocarbons (PAH) and their nitrogen analogs, basic azaarenes, are extracted from samples of airborne particulate matter by toluene with ultrasonic treatment. The basic azaarenes are extracted from the toluene phase with phosphoric acid, re-extracted from the phosphoric acid phase (adjusted to pH 14 with potassium hydroxide) with dichloromethane, and determined by capillary gas chromatography (g.c.) with a nitrogen-sensitive detector. The PAH in the toluene phase are isolated by means of semi-preparative high-performance liquid chromatography and liquid-liquid extraction and determined by g.c. with a flame-ionization detector. Eleven basic azaarenes were identified; their concentrations were one to two orders of magnitude lower than those of PAH. Results from the determination of the concentrations of basic azaarenes and PAH in the atmosphere in a busy street and in a suburban residential area of Copenhagen are presented and discussed.

BASIC RETENTION MECHANISMS
PART I: MULTIELEMENT ION-EXCHANGE.

Bror Skytte Jensen and Hanne Jensen.

European Appl. Res. Rept.- Nucl. Sci. Technol. 7 (1986) 481-538.

We have studied the effect of multiple cation competition on the adsorption of Sr onto two synthetic ion-exchange resins, i.e. DOWEX 50W and DOWEX CCR-2, as well as onto the clay mineral, kaolinite. Our results for DOWEX 50W, and under certain experimental conditions also for DOWEX CCR-2 were in good agreement with theoretical predictions for multielement ion-exchange[1] taking the limiting effect of ion-exchange capacity into account. In the case of very low cation adsorption, DOWEX CCR-2 showed an unexpected behaviour which is interpreted as ion-pair or ion-cluster adsorption of polyvalent ions. The data for kaolinite were similarly interpreted as adsorption of hydroxylated complexes of the polyvalent cations, a mechanism which has previously been suggested for the adsorption of heavy metals onto muds, sludges and organic debris.[3,4] In the case of kaolinite, indications of additional reactions like chemical transformations and dissolution reactions were observed. A single experimental point at higher Ca^{2+} concentrations showed a larger adsorption than expected from the general trend in data. A mass-transfer analysis indicates that under these experimental conditions Ca-smectites might be formed and therefore a Sr-Ca smectite as well. The outlier point may therefore well indicate the effect of a chemical transformation and therefore be a real effect.

The theoretical equations which have been confirmed by experiments are easily adaptable to modelling calculations. The experimental data were analysed by means of a computer program "MULTI-IONx", written for HP 9816, and is available on request.

COMPLEX FORMATION OF SELECTED RADIONUCLIDES WITH LIGANDS COMMONLY FOUND IN GROUND WATER:

LOW MOLECULAR ORGANIC ACIDS.

Bror Skytte Jensen and Hanne Jensen.

European Appl. Res. Rept.- Nucl. Sci. Technol. 6 (1985) 1477-1582.

A general approach to the analysis of potentiometric data on complex formation between cations and polybasic amphoteric acids is described. The method is used for the characterisation of complex formation between Cs^{+}, Sr^{2+}, Co^{2+}, La^{3+}, and Eu^{3+} with the α-hydroxy acids, tartaric acid and citric acid, and with the α-amino acids, aspartic acid and L-cysteine. The cations have been chosen as typical components of reactor waste, and the acids because they are often found as products of microbial activity in pits or wherever organic material decays.

For Cs^{+} there was no indication of complex formation as expected, and for Sr^{2+} only a weak complex with citric acid was characterised. All other cations investigated formed several complexes with the chosen ligands, many of them polynuclear and of complicated overall formulas.

Some of the data correspond well with older results from the literature, but species which have not been previously reported are identified and characterised in the majority of cases. Our results stress the need for a careful revaluation of older literature data before they are applied in modelling work.

The possible influence of complex formation on adsorption equilibria and thereby on the whole migration behaviour is discussed in a semiquantitative manner.

For all the systems investigated, predominance diagrams are derived, allowing for an easy identification of which complex species dominate under given conditions with regard to pH and total concentration of complexing acid.

During the studies, computer programs have been constructed allowing for 1) the characterisation of the acid dissociation constants for polybasic amphoteric acids, 2) the characterisation of the complex formation constants for any mixture containing species of the general formula $M_rA_xH_y(OH)_z$, and 3) programs used in displaying the predominance diagrams using the speciation constants determined by 1 and 2. The programs are written in HPL intended for 9816, 9825 or 9826 Hewlett-Packard desk-top computers with built-in matrix operations.

AIRBORNE HEAVY METAL POLLUTION IN THE ENVIRONMENT OF A DANISH STEEL PLANT.

N.K.Vestergaard, U.Stephansen, L.Rasmussen and K.Pilegaard.

Water, Air, and Soil Pollution. 27 (1986) 363-377.

A survey of heavy metal deposition was carried out in the vicinity of a Danish steel plant. Bulk precipitation and transplanted lichen (*Hypogymnia physodes* (L.) Nyl.) were sampled at 12 stations in the environment before and after the production had been converted from open-hearth furnaces to electric-arc furnaces. The samples were analyzed for Cd, Cr, Cu, Fe, Mn, Pb and Zn.

The results show that heavy metal pollution from the steelworks still is severe and that it follows a decreasing power curve when the distance to the steelworks is increased. However, a reduction in the deposition of heavy metals close to the steelworks has been observed, pointing to the conclusion that the change from a situation of emission through a 46 m stack without any filter to emission from the electric arc furnaces equipped with bag-filters has lead to changes in the emission. At the sampling stations with the highest deposition levels measured in bulk precipitation the corresponding concentrations in the lichens were relatively lower indicating a change in particle size distribution. Within each station there was a direct proportionality of metal concentrations in lichens and atmospheric fallout measured in bulk precipitation.

DIFFERENCES IN THERMAL STABILITY OF FROG AND RABBIT $\alpha\alpha$ - AND $\alpha\beta$ - TROPOMYOSINS DETERMINED BY OPTICAL ROTATORY DISPERSION.

Søren Hvidt.

Biophysical Chemistry. 24 (1986) 211-215.

Frog and rabbit $\alpha\alpha$- and $\alpha\beta$-tropomyosins were purified, and their thermal stabilities determined by use of optical rotatory dispersion. The tropomyosins were found to be virtually completely helical at 5°C. Regions of different thermal stabilities were seen for all tropomyosins. Rabbit and frog $\alpha\alpha$-tropomyosin show very similar thermal properties, with main transitions near 47-49°C. The main transition for frog $\alpha\beta$-tropomyosin is at 32°C. The results show that the $\alpha\beta$-tropomyosins are less stable than the $\alpha\alpha$-forms. Only thermal transitions of the $\alpha\beta$-forms appear to be correlated with the body temperatures of the animals.

OSCILLATORY MEASUREMENTS OF LINEAR VISCOELASTIC PROPERTIES OF SHEAR-THICKENING POLYMER SOLUTIONS.

Søren Hvidt, John D.Ferry and Robert F.Landel.

Journal of Rheology, 30 (1986) 43-54.

Measurements of dynamic viscoelastic properties in very small oscillating shear deformations have been made on solutions of a jet fuel, Jet A, containing an antimisting polymeric additive, FM-9. A few measurements were also made on solutions of FM-9 in a mixed solvent of mineral oil, tetralin, and o-terphenyl. Two samples of FM-9 had approximate number-average molecular weights of 12,000,000 and 8,100,000 as deduced from analysis of the measurements. The ranges of variables were 2.42–4.03 g/L in concentration (0.3 to 0.5% by weight), 1–35°C. in temperature, 1.3–9.4 cp in solvent viscosity, and 103–6100 Hz in frequency. Measurements in the Jet A solvent were made both with and without a modifying carrier. The results were compared with th. Zimm theory, and the viscoelastic behavior was found to resemble rather closely that of ordinary nonpolar polymers in Θ solvents. The relation of the results to the antithixotropic behavior of such solutions at high shear rates is discussed in terms of intramolecular and intermolecular interactions.

TEMPERATURE-DEPENDENT OPTICAL ROTATORY DISPERSION PROPERTIES OF HELICAL MUSCLE PROTEINS AND HOMOPOLYMERS.

Søren Hvidt, Michael E.Rodgers and William F.Harrington.

Biopolymers, 24 (1985) 1647-1662.

Thermally induced helix–coil transitions of myosin rod, light meromyosin, and tropomyosin were studied by optical rotatory dispersion (ORD). Fractional helicity was calculated from both the Moffitt-Yang parameter, b_0, and the corrected mean residue rotation $[m']$ at 231.4 nm. Between 3 and 30°C, $[m']$ increases linearly with a slope of 59/°C, whereas b_0 is virtually constant, indicating apparently different thermal melting behavior. Poly(L-lysine) and poly(L-glutamic acid) in their helical forms and myoglobin also show a nearly linear temperature dependence of $[m']_{231.4}$. Muscle proteins in 6*M* guanidine hydrochloride and the random-coil forms of the homopolymers exhibit temperature-dependent values of $[m']_{231.4}$ and b_0. We conclude from these observations that ORD properties of both α-helices and random-coil polypeptides have significant intrinsic temperature dependencies. A new method of estimating fractional helicity as a function of temperature is proposed.

OPTICAL PROPERTIES OF LARGE MOLECULES AND CLUSTERS IN THE FRENKEL EXCITON PICTURE.

John Avery and Søren Hvidt.

International Journal of Quantum Chemistry. 29 (1986) 497-510.

Frenkel exciton theory is reviewed. This theory yields general formulas relating the absorption and circular dichroism spectra of large molecules or clusters to the optical properties of their subunits. It is shown that for weakly interacting systems, the circular dichroism associated with a band of exciton states is proportional to tr(FH), where F is an "optical matrix" constructed from the positions and transition dipole moments of the subunits, and H is an interaction-energy matrix. It is shown that if a system expands isotropically, then tr(FH) falls off as the inverse square of the linear dimensions. This result is compared with experimental measurements of the low-temperature optical rotatory dispersion of proteins as a function of temperature. The optical properties of helical polymers are also discussed as a function of their geometrical parameters.

TVUNGEN KONTROL AF LÆGEUDSTYR KVALT I FØDSLEN.

V.N.Handlos.

Ingeniøren. 29/8-1986.

NOGLE TEKNISKE ASPEKTER VED GASSTERILISATION AF MEDICINSKE UTENSILIER.

Vagn Neerup Handlos.

Risø M-2592, 1986. ISBN 87-550-1241-8

The widespread application of sterilisation methods based on the use of gaseous sterilants at temperatures below 80 °C has enhanced the need for research in the field of the interaction between the gas and the sterilized items as well as the impact on the environment. Recent knowledge of the carcinogenic effects of the sterilants has actualized the need.

To avoid diffusion of the sterilants in medical devices, work places and environments it is imperative to gain knowledge of the reactivity of the sterilants, their deposition and transportation in various media.

The present thesis consisting of the preceding plus the enclosed 9 publications deals with technical problems of ethylene oxide and formaldehyde related to their usage as sterilants of medical devices in particular those made of plastic materials.

The description of the author's own work comprises:

- Data on solubility of ethylene oxide and formaldehyde in various plastic materials,
- Evaluation of methods to remove gas residues from sterilized goods including determination of diffusion coefficients for ethylene oxide and formaldehyde in a number of plastic materials.
- Explanation of formation of ethylene chlorohydrin in ethylene oxide sterilized polyvinylchloride,
- Description of formation of paraformaldehyde and their removal from sterilized goods,
- Design and development of equipment for formaldehyde sterilisation
- Measurement of airborne sterilants in the surroundings of ethylene oxide sterilisation plants and formaldehyde autoclaves,
- Development of a method and evaluation of existing methods of determination of gas residues in medical devices.

This part of the thesis is contained in the enclosed publications.

The first part of the thesis written in Danish (p.1-64) evaluates and gives an account of literature published within the subject. An attempt to establish relations between toxicological data and the author's technical results is made. Further, official limits of gas residues in sterilized products are suggested and a recommendation is put forward to the National Agency for Environmental Protection in Denmark to take action.

DETERMINATION OF THE EQUILIBRIUM CONSTANT FOR THE TAUTOMERIC 9-HYDROXYANTHRACENE/9-ANTHRONE SYSTEM IN APROTIC SOLVENTS BY A NOVEL APPLICATION OF CYCLIC VOLTAMMETRY.

Kristoffer Almdal, Hanne Eggert and Ole Hammerich.

Acta Chemica Scandinavica B 40 (1986) 230-232.

Short Communication.

THE STRUCTURE OF THE LOWEST EXITED TRIPLET STATES OF HEXATRIENES STUDIED BY TIME-RESOLVED RESONANCE RAMAN SPECTROSCOPY.

Frans W.Langkilde, Niels-Henrik Jensen, Robert Wilbrandt, Albert M.Brouwer and Harry J.C.Jacobs.

in XI IUPAC Symposium on Photochemistry,Abstracts, Lisbon, (1986) 77-78.

THE STRUCTURE OF THE LOWEST EXITED TRIPLET STATES OF HEXATRIENES STUDIED BY TIME-RESOLVED RESONANCE RAMAN SPECTROSCOPY.

F.W.Langkilde, N-H.Jensen, R.Wilbrandt, A.M.Brouwer and H.J.C.Jacobs.

in Proceedings of the Xth International Conference on Raman Spectroscopy, Eugene, Oregon, (1986) Chapter 18. pp. 16-17.

ABSOLUTE RATE CONSTANT FOR THE REACTION OF OH WITH SO_2 IN THE PRESENCE OF WATER AT ATMOSPHERIC PRESSURE.

O.J.Nielsen, P.Pagsberg and A.Sillesen.

in Psysico-Chemical Behaviour of Atmospheric Pollutants. Proceedings of the 4th European Symposium. Stresa (1986) 472-478.

The gas phase reaction of OH with SO_2 in the presence of water was studied at atmospheric pressure. OH radicals were produced by pulse radiolysis of water/Ar mixtures. The formation and decay of OH were followed by monitoring the transient light absorbtion at 309 nm. $k(OH+SO_2)$ in the presence of water at 10 mbar was determined to 0.8×10^{-12} $cm^3 molec^{-1} s^{-1}$. A search for the absorption spectrum of the HSO_3 radical has not yet been succesful.

PHOTO-OXIDATION OF SULPHUR CONTAINING COMPOUNDS.

O.J.Nielsen, P.Pagsberg, J.Treacy, L.Nelson and H.Sidebottom.

in Psysico-Chemical Behaviour of Atmospheric Pollutants. Proceeding of the 4th European Symposium. Stresa (1986) 385-391.

The reactions of OH with dimethyldisulfide (DMDS), dimethylsulfide (DMS), and diethylsulfide (DES) have been investigated applying both a photolytic relative technique and an absolute method using pulse radiolysis combined with kinetic spectroscopy. Furthermore, the reactions of OH with di-tert-butyldisulfide (DTBDS), ethylpropylsulfide (EPS), and dipropylsulfide (DPS) were studied using the absolute method. All measurements were done at room temperature and atmospheric pressure. The relative method using methyl nitrite as OH source was found to give unreliable OH rate constants with organic sulfides. The following absolute OH rate constants were obtained:

$$k(OH + DMDS) = (300 \pm 30) \times 10^{-12}$$
$$k(OH + DTBDS) = (41 \pm 4) \times 10^{-12}$$
$$k(OH + DMS) = (3.5 \pm 0.4) \times 10^{-12}$$
$$k(OH + DES) = (4.5 \pm 0.5) \times 10^{-12}$$
$$k(OH + EPS) = (4.9 \pm 0.5) \times 10^{-12}$$
$$k(OH + DPS) = (5.2 \pm 0.5) \times 10^{-12}$$

(units are $cm^3 molecule^{-1} s^{-1}$)

The data for the sulfides are consistent with the concept of group rate constants. The relative measured rate constants for the reaction of OH with DMS and DFS were found to increase with increasing concentrations of added NO. These results provide some indication of the reasons for the difference in reported rate constants for these reactions.

REACTIONS OF HYDROXYL RADICALS WITH SULPHUR CONTAINING COMPOUNDS.

P.Pagsberg, O.J.Nielsen, J.Treacy, L.Nelson and H.Sidebottom.

in 9th International Symposium on Gas Kinetics. Bordeaux. (1986) I-32.

Biogenic and anthropogenic emissions of sulphur compounds are thought to be about equal. In order that the contribution of anthropogenic emissions to acid deposition can be precisely defined it is clear that an understanding of the natural sulphur cycle is desirable. Reduced sulphur compounds such as H_2S, CS_2, CH_3SCH_3 and CH_3SSCH_3 are considered to be the most important biogenic sources of sulphur in the troposphere. These compounds are thought to be oxidized by homogeneous reactions involving hydroxyl radical initiated processes, however detailed reaction mechanisms remain obscure. Numerous experimental studies have been reported concerning the kinetics of these reactions, however, there is often conflict between rate constant data determined using absolute methods at low pressure and relative techniques under simulated atmospheric conditions.

ABSOLUTE RATE CONSTANTS FOR THE GAS-PHASE REACTION OF OH RADICALS WITH CYCLOHEXANE AND ETHANE AT 295 K

Ole J.Nielsen, Jette Munk, Palle Pagsberg and Alfred Sillesen.

Chemical Psysics Letters. 128 (1986) 168-171.

The absolute rate constants for the gas-phase H-atom abstraction by hydroxyl radicals from cyclohexane and ethane have been determined at room temperature. OH radicals were produced by pulse radiolysis of an H_2O-Ar mixture, and the decay of OH was followed by monitoring the transient light absorption around 309 nm. The rate constants were found to be $k = (5.24 \pm 0.36) \times 10^{-12}$ and $(2.98 \pm 0.21) \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} for cyclohexane and ethane, respectively. These results are compared with literature data.

PHOTO-OXIDATION OF SULPHUR CONTAINING COMPOUNDS.

P.Pagsberg, O.J.Nielsen, J.Treacy, L.Nelson and H.Sidebottom.

in European Science Foundation Workshop on Tropospheric Ozone Chemistry. Dubrovnik. (1986) 385-391. P 12.

Reactions of sulphur containing compounds in the troposphere are of importance since the reaction products contribute to sulphuric acid and aerosol formation. The dominant homogenous removal pathways for these sulphur species are initiated by reaction with hydroxyl radicals, however, detailed reaction mechanisms for many of the reactions remain obscure. Numerous experimental studies have been reported concerning the kinetics of these reactions, however, there is often conflict between rate constant data determined using absolute methods at low pressure and relative techniques under simulated atmospheric conditions. This work is concerned with the determination of rate constants and mechanism for the reaction of hydroxyl radicals with sulphur dioxide and a number of reduced sulphur containing compounds under atmospheric conditions. The reactions were studied using both a relative rate method and the technique of pulse radiolysis combined with kinetic spectroscopy. It was hoped that the results would provide some indication of the reasons for the differences in the reported rate data for these reactions.

SPECTROKINETIC STUDIES OF VINYL RADICALS.

Jette Munk, P.Pagsberg, E.Ratajczak and A.Sillesen.

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Vinyl Radicals were produced via different source reactions initiated by pulse radiolysis of H_2/C_2H_2, Ar/C_2H_3Cl or $Ar/1,3\text{-}C_4H_6$, i.e.

(1) $H + C_2H_2 + M \rightarrow C_2H_3 + M$

(2) $Ar^* + C_2H_3Cl \rightarrow Ar + C_2H_3 + Cl$

(3) $Ar^* + CH_2{=}CH\text{-}CH{=}CH_2 \rightarrow Ar + 2\ C_2H_3$

The ultraviolet absorption band of C_2H_3 with a maximum at 210 nm which was observed in the present investigation has not been reported previously. The overall rate constant for the self reaction has been determined from the observed transient absorption signals and work is in progress to determine the branching ratio, k_{4a}/k_{4b} for the product channels

(4a) $2\ C_2H_3\ (+M) \rightarrow 1,3\text{-}C_4H_6\ (+M)$

(4b) $2\ C_2H_3 \rightarrow C_2H_4 + C_2H_2$.

Based on the observed spectral features and the kinetics of the self reaction we want to study the reaction $C_2H_3 + O_2 \rightarrow$ products which may also proceed via two different exothermic channals.

SPECTROKINETIC STUDIES OF i-C_3H_7 AND i-$C_3H_7O_2$ RADICALS.

Jette Munk, Palle Pagsberg, Emil Ratajczak and Alfred Sillesen.

Chemical Physics Letters. 132 (1986) 417-421.

UV absorption spectra of *i*-C_3H_7 and *i*-$C_3H_7O_2$ radicals have been obtained following pulse radiolysis of H_2/C_3H_8 and $H_2/C_3H_8/O_2$ mixtures at a total pressure of 1 atm at room temperature. The *i*-C_3H_7 spectrum shows two absorption maxima with $\epsilon(233\ nm) = 890 \pm 130\ M^{-1}\ cm^{-1}$ and $\epsilon(205\ nm) = 780 \pm 120\ M^{-1}\ cm^{-1}$, respectively. The spectrum of *i*-$C_3H_7O_2$ is a broad continuum with a maximum of $\epsilon = 1300 \pm 200\ M^{-1}\ cm^{-1}$ at 223 nm. By computer-aided analysis of the kinetic features a consistent set of rate constants for the reactions involved in these systems have been deduced.

SPECTROKINETIC STUDIES OF ETHYL AND ETHYLPEROXY RADICALS.

Jette Munk, Palle Pagsberg, Emil Ratajczak and Alfred Sillesen.

The Journal of Physical Chemistry. 90 (1986) 2752-2757.

Hydrogen atoms were produced by pulse radiolysis of H_2 at 1 atm and $T = 298$ K. The yield of H atoms was determined by monitoring the UV absorption of HO_2 produced in the presence of oxygen via the reaction $H + O_2 (+M) \rightarrow HO_2 (+M)$. In the presence of small amounts of C_2H_4 we observed the formation of ethyl radicals via $H + C_2H_4 (+M) \rightarrow C_2H_5 (+M)$ (6) as well as the subsequent decay via $2C_2H_5 \rightarrow C_4H_{10}, C_2H_4 + C_2H_6$ (8). The spectrum of C_2H_5 is composed of two absorption bands with maxima at 205 and 245 nm. The 205-nm band exhibits a characteristic fine structure with a maximum extinction coefficient of $2010 \pm 300\ M^{-1}\ cm^{-1}$. The weaker 245-nm band appears to be a broad continuum with an extinction coefficient of $870 \pm 130\ M^{-1}\ cm^{-1}$. By computer-aided analysis of the kinetic features we have obtained values of $k_6 = (5.5 \pm 0.5) \times 10^8\ M^{-1}\ s^{-1}$ and $2k_8 = (2.3 \pm 0.3) \times 10^{10}\ M^{-1}\ s^{-1}$. In the presence of both C_2H_4 and O_2 we observed the formation of ethylperoxy radicals, $C_2H_5 + O_2 (+M) \rightarrow C_2H_5O_2 (+M)$ (10a), followed by a slow second-order decay, $2C_2H_5O_2 \rightarrow$ products (13). The spectrum of $C_2H_5O_2$ is a broad continuum with a maximum at 230 nm and $\epsilon = 1410 \pm 200\ M^{-1}\ cm^{-1}$. From the observed rate of formation we obtained $k_{10a} = (3.2 \pm 0.1) \times 10^9\ M^{-1}\ s^{-1}$ at $p(M) = p(H_2) = 1$ atm. From the observed second-order decay we have determined $2k_{13} = (6.3 \pm 0.3) \times 10^7\ M^{-1}\ s^{-1}$. The rate of reaction 10a was studied in the range of 298–400 K, and the results may be presented in terms of an Arrhenius expression with an apparent negative activation energy, $\log k_{10a}/M^{-1}\ s^{-1} = (8.90 \pm 0.04) + (840 \pm 70)\ cal\ mol^{-1}/2.303RT$.

ON Ps FORMATION IN MODERATELY DENCE MOLECULAR GASES.

Finn M.Jacobsen.

Chemical Physics 109 (1986) 455-464.

Positronium, Ps, formation as a result of the so-called Ore, Ore/spur-like, and spur processes in molecular gases is discussed in the density range from 1 to about 50 amagat. Semi-quantitatively, it is possible to explain much of the density and temperature dependence of the Ps fraction experimentally observed. Phenomena such as the formation of energetic Ps, breakup of energetic Ps followed by recombination to form "stable" Ps, Ps formed as a result of spur processes and mobilities of excess electrons and of the positron take their natural part in the interpretation of Ps fractions in molecular gases.

ON POSITRONIUM FORMATION IN CRYSTALLINE AND AMORPHOUS ICE AT LOW POSITRON ENERGY.

O.E.Mogensen.

Physics Letters A. 118 (1986) 357-362.

The positronium (Ps) yield for ice, measured by Eldrup et al. using a low-energy positron beam, is discussed in terms of the spur model of Ps formation. The pronounced maxima in the Ps yield for crystalline ice at positron energies below 6.5 eV are well explained by effects due to energy conservation in the spur processes. Parts of the amorphous ice results are well explained by the spur but not by the Ore model. Important processes influencing the Ps formation are not included in the Ore model.

POSITRONIUM FORMATION AND HYDRATED POSITRON REACTIONS IN H_2O, D_2O, 1.74 M PPS/H_2O AND 1.74 M PPS/D_2O SOLUTIONS OF Cl^-, Br^- AND I^-.

O.E.Mogensen and N.J.Pedersen.

Radiat.Phys.Chem. 28 (1986) 33-48.

Angular correlation of annihilation photons were measured for H_2O, D_2O, 1.74 M PPS/H_2O and 1.74 M PPS/D_2O solutions of Cl^-, Br^- and I^-. The three components of the angular correlation spectra for D_2O and H_2O were nearly identical in shape. The positronium (Ps) yields for the H_2O and D_2O solutions, extracted from the angular correlation spectra, were somewhat different from those extracted previously from the lifetime spectra. Positrons form bound states $[X^-, e^+]$ with Cl^-, Br^- and I^-, but not with acetate, oxalate, SO_4^{2-}, OH^- and F^- ions, in water. The percentage of positron bound state formation before annihilation (lifetime 400 ps) was determined for the three halides in the four solvents. Simple kinetic equations ("trapping model") with time dependent rate constant, solved analytically, could explain the $[X^-, e^+]$ formation in H_2O fairly well for concentrations below 0.03 M X^-, if a diffusion controlled reaction with positron diffusion constant $D = 5 \times 10^{-5}$ cm^2/s and reaction radius $R = 1$ nm were assumed. The three halides gave roughly identical $[X^-, e^+]$ formation below 0.03 M X^-. The difference between the four solutions could be explained partly only in terms of viscosity change for the model used. The effective rate constant decreased strongly for increasing X^- concentration above 0.03 M X^-. Ion association may influence the e^+_{th} reaction. The high concentration results are very difficult to explain.

MUONIUM FORMATION IN NONPOLAR LIQUIDS.

O.E.Mogensen and P.W.Percival.

Radiat.Phys.Chem. 28 (1986) 85-89.

Despite the very wide acceptance of the spur model of positronium formation there has been continuing criticism of the analogous model for muonium formation. After critical comparison of the muonium and positronium formation processes it is shown how differences in muonium and positronium behaviour can be explained by differences in their properties and the way in which measurements are made. It is concluded that the sparse data presently available for muonium are consistent with a spur formation process.

LECTURES and POSTERS

1.1 K. Heydorn: "Neutron Transmutation Doping of Silicon at Risø National Laboratory". IAEA Consultants' Meeting on Silicon Transmutation Doping Techniques and Practices. Otwock-Swierk, Polen, 21st November 1985.

1.2 K. Heydorn: "Interne Serviceydelser på Risø". Risøs Lederudviklingsprogram LUP-86. Klarskovgaard, Korsør, 3rd March 1986.

1.3 K. Heydorn: "Neutronaktiveringsanalyse". Dansk Ingeniørforening, Copenhagen, 9th October 1986.

1.4 K. Heydorn: "Certification Analyses of Reference Materials". BCR-Informationsmøde. Teknologistyrelsen, Copenhagen, 6th November 1986.

1.5 K. Heydorn: "Metoder til Bestemmelse af Se". Arbejdsmøde om Sporstofforskning, Århus, 17th November 1986.

1.6 K. Heydorn: "Modern Applications of Neutron Activation Analysis for Biological Materials". Symposium om Nukleäre Analysmetoder. Stockholm, 20th November 1986.

1.7 Else Damsgaard and K. Heydorn: "Synthesis of Precision for the Certification of Phosphorus in Biological Materials by INAA". 7th International Conference MTAA. Copenhagen, 23rd-27th June 1986.

1.8 Leif Højslet Christensen and K. Heydorn: "Quality Assurance in the Determination of Overlapping Peak Areas". 7th International Conference MTAA. Copenhagen, 22rd-27th June 1986.

1.9 H.K. Nielsen and J.O. Schmidt: "Instrumental Neutron Activation Analysis Technique Using Subsecond Radionuclides". 7th International Conference MTAA. Copenhagen, 22rd-27th June 1986.

2.1 Elfinn Larsen: "Long-Term Stability of a GC-MS System in Quantitative Gas Analyses". The 6th Nordic Conference on Mass Spectrometry. Øland, Sverige, 25th-28th May 1986.

2.2 Helge Egsgaard, Lars Carlsen and Susanne Elbel: "Isomerization of the Nitromethane Radical Cation in the Gas Phase". The 6th Nordic Conference on Mass Spectrometry. Borgholm, Øland, Sverige, 25th-28th May 1986.

2.3 Helge Egsgaard: "Low-Pressure Pyrolysis/Mass Spectrometry. Strategies for Disclosing Reaction Pathways". Dansk Massespektrometrisk Selskab. Odense, 27th August 1986.

2.4 Helge Egsgaard, Peter Bo and Lars Carlsen: "Intramolecular Isotope Distribution Derived Directly from the Ion Pattern". Dansk Massespektrometrisk Selskab. Odense, 27th August, 1986.

2.5 Lars Carlsen and Helge Egsgaard: "Gas Phase Pyrolysis of Methyl N,N-Dimethylcarbamate and the Corresponding Mono- and Dithioderivatives". Contribution to the 12th International Symposium on the Organic Chemistry of Sulfur. Nijmegen, July 1986.

2.6 Lars Carlsen and Helge Egsgaard: "The Fate of Molecules in Low Pressure Pyrolysis Reactors". Contribution to 7th International Symposium on Analytical and Applied Pyrolysis. Reading, September 1986.

2.7 K.E. Andersen and Lars Carlsen: "Triphenyl Phosphate Allergy from Spectacle Frames, Chemical Analyses and Patch Test Results in one Patient". Contribution to 8th International Symposium on Contact Dermatitis. Cambridge, March 1986.

3.1 Lars Carlsen: "Basic Research in Migration Studies". Lecture at Battelle Northwest Laboratories. Richland, November 1986.

3.2 Torben Nielsen: "Partikulære Organiske Forbindelser: Forekomst og Atmosfærekemi". Atmosfærekemisk Colloquium. Planlægningsrådet for Forskningen. Risø, 18th April 1986.

3.3 K. Pilegaard: "Kritisk Gennemgang af NMR-MIL 3 Projektet: Försurningens Inverkan på Metalltransport i Miljön". NMR -Seminarium om Miljöeffekter av Energiproduktion. Stockholm, 27th-28th Maj 1986.

3.4 O.J. Nielsen, P. Pagsberg, J. Treacy, L. Nelson, and H. Sidebottom: "Photooxidation of Sulphur Containing Compounds". European Science Foundation Workshop on Tropospheric Ozone Chemistry. Dubrovnik, 11th-17th May 1986.

3.5 O.J. Nielsen, J. Treacy, L. Nelson, and H. Sidebottom: "Reaction of Hydroxyl Radicals with Sulphur Containing Compounds". 9th International Symposium on Gas Phase Kinetics. Bordeaux, 20th-25th July 1986.

3.6 O.J. Nielsen, J. Treacy, L. Nelson, and H. Sidebottom: "Photooxidation of Sulphur Compounds". 4th European Symposium on Physico-Chemical Behaviour of Atmospheric Pollutants. Stresa, 23rd-25th September 1986.

3.7 O.J. Nielsen, P. Pagsberg and A. Sillesen: "Absolute Rate Constant for the Reaction of OH with SO_2". 4th European Symposium on Physico-Chemical Behaviour of Atmospheric Pollutants. Stresa, 23rd-25th September 1986.

4.1 V.N. Handlos: "Påvirkning af polymerer ved strålesterilisation". Polymerteknisk Selskab. Risø, 13th March 1986.

4.2 V.N. Handlos: "Medicinsk anvendte phthalater". Kemisk Forening. H.C.Ø., Copenhagen, 26th May 1986.

4.3 V.N. Handlos: "Plastics Monographs in the European Pharmacopoeia". Pharmaceutical Inspectors Convention. Sigtuna, Sweden, 17th June 1986.

4.4 V.N. Handlos: "Pharmaceutical Sterilisation of Plastics". Pharmaceutical Inspectors Convention. Sigtuna, Sweden, 18th June 1986.

4.5 S. Hvidt: "Conformational Changes in Tropomyosin". Dept. of Biology, The Johns Hopkins University, Baltimore, USA, 9th July 1986.

4.6 W. Batsberg: "Størrelseschromatografisk analyse af syntetiske og biologiske polymerer". Analytikerringen. DFH, Copenhagen, 21st August 1986.

4.7 W. Batsberg: "Præparative anvendelser af væskechromatografiske teknikker". Analytikerringen. DFH, Copenhagen, 21st August 1986.

4.8 S. Hvidt, O. Kramer, W. Batsberg: "Kædebevægelser i lineære og tredimensionale polymerer". FTU-seminar. DTH, Lyngby, 27th August 1986.

4.9 V.N. Handlos, S. Hvidt, W. Batsberg: "Strukturer af makromolekyler i vandig opløsning". FTU-seminar. DTH, Lyngby, 27th August 1986.

4.10 K. Mortensen, O. Kramer, W. Batsberg, and L.J. Fetters: "Polymer Coil Relaxation in Uniaxial Strained Polybutadiene observed by Small Angle Neutron Scattering". Networks 86, Elsinore, 2nd September 1986.

4.11 W. Batsberg, S. Hvidt, O. Kramer and L.J. Fetters: "High -Vinyl-Polybutadiene Cross-linked in the Strained State to different Degrees of Crosslinking". Networks 86, Elsinore, 2nd September 1986.

4.12 V.N. Handlos: Mundtligt forsvar af doktorafhandlingen: "Nogle tekniske aspekter ved gassterilisation af medicinske utensilier". Danmarks Farmaceutiske Højskole, Copenhagen, 12th September 1986.

4.13 V.N. Handlos: "Plastmaterialers egnethed for sterilisation med gas-, stråling- og termiske sterilisations metoder". R^3-foreningens højere grundkursus, Holte, 29th October 1986.

4.14 S. Hvidt: "Domain Structures in Myosins". Physics in Biology. DTH, Lyngby, 12th November 1986.

4.15 V.N. Handlos: "Transport af sterilisationsgasser i Plast". Polymerteknisk Selskab. H.C.Ø., Copenhagen, 20th November 1986.

4.16 S. Hvidt: "Struktur og funktion af proteiner". Folkeuniversitetet i Roskilde, 22nd November 1986.

4.17 K. Mortensen, O. Kramer, W. Batsberg, L.J. Fetters: " Coil Relaxation in Uniaxially Deformed Polymer Melt". Materials Research Society Symposium. Oak Ridge, USA, 2nd December 1986.

4.18 V.N. Handlos: "Zur Gassterilisation in Skandinavischen Krankenhäusern", Medizinische Universität zu Lübeck, Lübeck, 17th December 1986.

5.1 R. Wilbrandt: "The Structure of the lowest Excited Triplet States of Hexatrienes". First Nordic Workshop on Photochemistry. Uppsala, Sweden, 26th August 1986.

5.2 R. Wilbrandt: "The Structure of the lowest Excited Triplet States of Hexatrienes". Gordon Conference. Vibrational Spectroscopy. Wolfeboro, New Hampshire, USA, 12th August 1986.

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This report contains a brief survey of the main activities in the Chemistry Department. All articles and reports published and lectures given in 1986 are presented. The facilities and equipment are mentioned briefly. The activities are divided into the following groups: radioisotope chemistry, analytical- and organic chemistry, environmental chemistry, polymer chemistry, radical chemistry, mineral processing, and general.

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